#13 Raspršenje elektromagnetskih valova na kristalima

I Dipolno zračenje

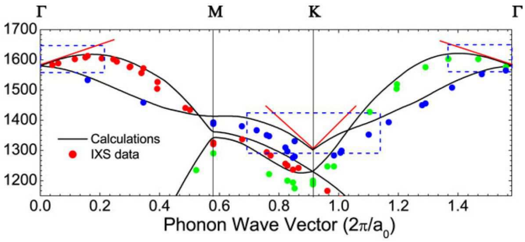
II Raspršenje vidljive svjetlosti i X zraka

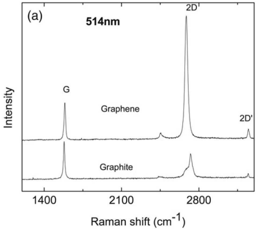
predavanja 20**

Motivacija I

karakteristični eksperimentalni rezultati u grafenu

- neelastično raspršenje X zraka [Maultzsch *et al.*, 2007]
- ramansko raspršenje (vidljive svjetlosti) [Ferrari, 2007]

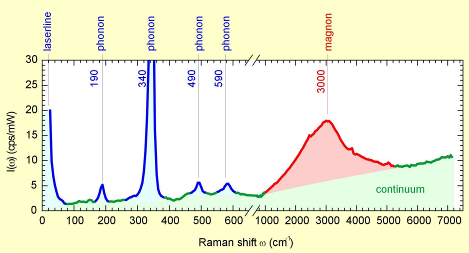


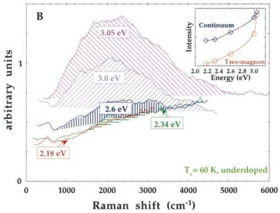


Motivacija I

karakteristični eksperimentalni rezultati u visokotemperaturnim supravodičima

- elektronsko, fononsko i dvomagnonsko ramansko raspršenje u B_{1g} kanalu [Devereaux, Hackl, 2007]
- rezonantno dvomagnonsko raspršenje [Blumberg *et al.*, 1997]





Geometrija problema

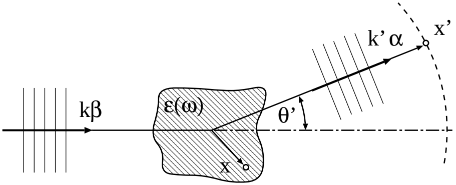
što i kako mjerimo?

- mjerimo udarni presjek u zoni radijacije

$$\sigma = \int \mathrm{d}\Omega' \left(\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega'}\right), \qquad \frac{\mathrm{d}\sigma}{\mathrm{d}\Omega'} = C\,\frac{r'^2\langle|\mathbf{E}'|^2\rangle}{|\mathbf{E}|^2}$$

- teorijski opis pomoću dielektričnog pomaka

$$D'_\alpha(\mathbf{x}',\omega') = \varepsilon'(\omega')E'_\alpha(\mathbf{x}',\omega') + \sum_\beta \delta\varepsilon_{\alpha\beta}(??)E_\beta(\mathbf{x}',\omega)$$



Redefinicija pojma točke

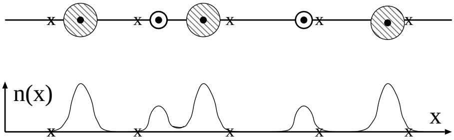
raspršenje em valova u mikroskopskoj fizici čvrstog stanja

- definicija kvantnomehaničke gustoće naboja

$$\rho_m(\mathbf{x},t) \approx \sum_{nl} z_l e \delta(\mathbf{x}-\mathbf{x}_{nl}(t)) + n(\mathbf{x},t), \quad n(\mathbf{x},t) = \sum_{nl} n_l(\mathbf{x}-\mathbf{x}_{nl}(t))$$

- 'mikroskopska' točka $\mathbf{x}$ (vrijedi i u makroskopskoj granici!)
- gustoća naboja elektrona u ravnoteži

$$n_0(\mathbf{x}) = \sum_m \mathrm{e}^{i\mathbf{K}_m\cdot\mathbf{x}}\, n_0(\mathbf{K}_m)$$



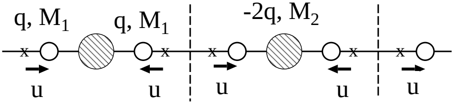
Fluktuacije naboja

$\mathbf{k} \approx 0$ *monopolne*, *dipolne i* *kvadrupolne* *fluktuacije naboja*

- fluktuacije gustoće vodljivih i vezanih elektrona u teoriji raspršenja

$$\delta n(\mathbf{x}, t) = n(\mathbf{x}, t) - n_0(\mathbf{x}) \approx \sum_{nl} \mathbf{u}_{nl}(t) \cdot \nabla_{\mathbf{x}_{nl}} \sum_{n'l'} n_{n'l'}(\mathbf{x}; \{\mathbf{x}_{nl}\})$$

- u ramanskom raspršenju: $\mathbf{k} \approx 0$ kvadrupolne fluktuacije naboja $\delta n_{\alpha\beta}(\mathbf{x}, t)$ [dipolno izborno pravilo]
- u difrakciji X zraka: ravnotežna gustoća elektrona $n_0(\mathbf{x})$



Dielektrični pomak

- polja u klasičnoj teoriji raspršenja

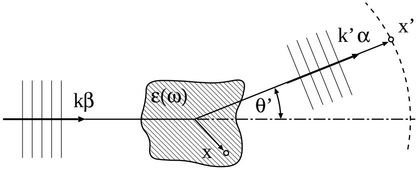
$$\mathbf{E} \equiv \mathbf{E}(\mathbf{x}, \omega), \quad \mathbf{E}' \equiv \mathbf{E}(\mathbf{x}, \omega'), \quad \mathbf{D}' \equiv \mathbf{D}(\mathbf{x}, \omega')$$

- dielektrični pomak $[\mathbf{D}' = \varepsilon' \, \mathbf{E}' + \delta\hat{\varepsilon} \, \mathbf{E}]$

$$\mathbf{D}' = \sum\nolimits_{\alpha} D'_{\alpha} \hat{e}_{\alpha}, \quad D'_{\alpha} = \varepsilon' E'_{\alpha} + \sum\nolimits_{\beta} \delta\varepsilon_{\alpha\beta} E_{\beta}$$

- klasična 'teorija' raspršenja $[\varepsilon(\mathbf{x}, \omega) = 1 - (4\pi e^2/m\omega^2) n(\mathbf{x}, \omega)]$

$$\delta\varepsilon_{\alpha\beta}(\mathbf{x}, \omega, \omega') = \frac{4\pi e^2}{m\omega\omega'} \delta n_{\alpha\beta}(\mathbf{x}, \omega, \omega')$$



Dipolno zračenje u klasičnoj elektrodinamici

kako izgledaju električna i magnetska komponenta polja u zoni radijacije?

- Maxwellove jednadžbe [$\mu = \mu' = 1$ i $\omega'/c = k'$]

$$\nabla \cdot \mathbf{D}'(\mathbf{x}, t) = 0, \qquad \nabla \times \mathbf{E}'(\mathbf{x}, t) = ik'\mathbf{H}'(\mathbf{x}, t)$$
$$\nabla \cdot \mathbf{H}'(\mathbf{x}, t) = 0, \qquad \nabla \times \mathbf{H}'(\mathbf{x}, t) = -ik'\mathbf{D}'(\mathbf{x}, t)$$

- pojednostavljena forma jednadžbi

$$\nabla \cdot \mathbf{E}' \approx 0, \qquad \nabla \times \mathbf{E}' = ik'\mathbf{H}'$$
$$\nabla \cdot \mathbf{H}' = 0, \qquad \nabla \times \mathbf{H}' = -ik'\varepsilon'\mathbf{E}' + (4\pi/c)\mathbf{J}$$

- uz efektivni strujni izvor

$$\mathbf{J}(\mathbf{x}, t) = -i(\omega'/4\pi)\delta\hat{\varepsilon}(\mathbf{x}, t)\,\mathbf{E}(\mathbf{x}, t) \equiv -i(e^2/m\omega)\delta\hat{n}(\mathbf{x}, t)\,\mathbf{E}(\mathbf{x}, t)$$

Dipolno zračenje u klasičnoj elektrodinamici

rješenje

- ukupni dipolni moment

$$\mathbf{P}(t) = \frac{i}{\omega'} \int_V \mathrm{d}^3x \, \mathrm{e}^{-i\mathbf{k}'\cdot\mathbf{x}} \mathbf{J}(\mathbf{x}, t) = \int_V \mathrm{d}^3x \, \mathrm{e}^{-i\mathbf{k}'\cdot\mathbf{x}} \frac{e^2 \delta\hat{n}(\mathbf{x}, t)}{m\omega\omega'} \, \mathbf{E}(\mathbf{x}, t)$$

- rješenje u zoni radijacije

$$\mathbf{A}' = -ik'\mathbf{P}(\mathrm{e}^{ik'r'}/cr'), \quad \mathbf{H}' = \nabla \times \mathbf{A}', \quad \mathbf{E}' = k'^2 \big(\mathbf{n} \times \mathbf{P}\big) \times \mathbf{n} \, (\mathrm{e}^{ik'r'}/r')$$

- fluktuacije naboja

$$\delta\mathbf{n}(-\mathbf{q}) = \int \mathrm{d}^3x \, \mathrm{e}^{i\mathbf{q}\cdot\mathbf{x}} \delta\hat{n}(\mathbf{x}) \, \hat{e}_\beta, \quad \big|\big(\mathbf{n} \times \delta\mathbf{n}\big) \times \mathbf{n}\big| = \delta n_\perp$$

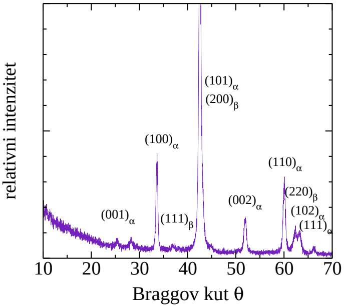
- električna komponenta polja

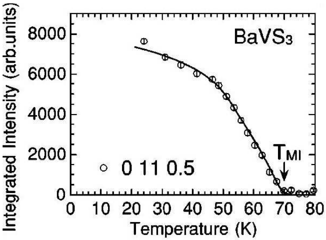
$$\mathbf{E}' = E_0 \mathrm{e}^{-i\omega' t} \frac{k'}{k} \frac{e^2}{mc^2} \delta n_\perp(-\mathbf{q}) \, \frac{\mathrm{e}^{ik'r'}}{r'} \hat{e}_\alpha$$

Motivacija II

difrakcija X zraka (elastično raspršenje X zraka)

- u supravodiču MgB_2 [Skoko *et al.*, 2010]
- u sustavu s valovima gustoće naboja $BaVS_3$ [Inami *et al.*, 2002]





Udarni presjek

. . . za raspršenje em valova na kristalima

- Fourierov transformat korelacijske funkcije između gustoća naboja

$$\langle n(\mathbf{q}, t_1) n^*(\mathbf{q}, t_2) \rangle = \int_V \mathrm{d}^3 x_1 \int_V \mathrm{d}^3 x_2 \, \mathrm{e}^{-i\mathbf{q}\cdot(\mathbf{x}_1 - \mathbf{x}_2)} \langle n(\mathbf{x}_1, t_1) n^*(\mathbf{x}_2, t_2) \rangle$$

- statička korelacijska funkcija $[\langle nn^* \rangle_{\mathbf{q}} = \int \mathrm{d}^3 x \, \mathrm{e}^{-i\mathbf{q}\cdot\mathbf{x}} \langle n(\mathbf{x}) n^*(0) \rangle]$

$$\langle n(\mathbf{q}) n^*(\mathbf{q}) \rangle = \langle |n(\mathbf{q})|^2 \rangle = V \langle nn^* \rangle_{\mathbf{q}}$$

- udarni presjek

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega'} = \frac{k'}{k} \left(\frac{e^2}{mc^2} \right)^2 \langle |n_\perp(\mathbf{q})|^2 \rangle \approx \left(\frac{e^2}{mc^2} \right)^2 \frac{1}{2} (1 + \cos^2 \theta') \langle |n(\mathbf{q})|^2 \rangle$$

Udarni presjek razlučiv po energijama

- korelacijska funkcija za različita vremena

$$\frac{\mathrm{d}\sigma_{\alpha\beta}(t_1, t_2)}{\mathrm{d}\Omega'} = \frac{r'^2 k}{k'} \left\langle \frac{E'_\beta(t_1)}{E_\alpha(t_1)} \frac{E'^*_\beta(t_2)}{E^*_\alpha(t_2)} \right\rangle$$

- udarni presjek

$$\frac{\mathrm{d}\sigma_{\alpha\beta}}{\mathrm{d}\Omega'} = \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega_0}{2\pi} \frac{\mathrm{d}\sigma_{\alpha\beta}}{\mathrm{d}\Omega' \mathrm{d}\omega_0} \Rightarrow \frac{\mathrm{d}\sigma_{\alpha\beta}}{\mathrm{d}\Omega' \mathrm{d}\omega_0} = \int_{-\infty}^{\infty} \mathrm{d}t_1 \, \mathrm{e}^{i\omega_0 t_1} \frac{\mathrm{d}\sigma_{\alpha\beta}(t_1, 0)}{\mathrm{d}\Omega'}$$

- ... razlučiv po energijama (za kvadrupolne fluktuacije)

$$\frac{\mathrm{d}\sigma_{\alpha\beta}}{\mathrm{d}\Omega' \mathrm{d}\omega_0} = \frac{k'}{k} \left(\frac{e^2}{mc^2} \right)^2 V \langle \delta n_{\alpha\beta} \delta n^*_{\alpha\beta} \rangle_{\mathbf{q}\,\omega_0}$$

Fononsko ramansko raspršenje

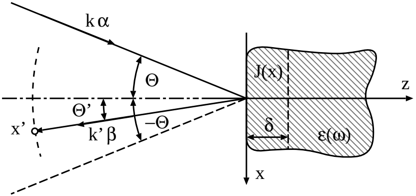
izborna pravila u ramanskom raspršenju

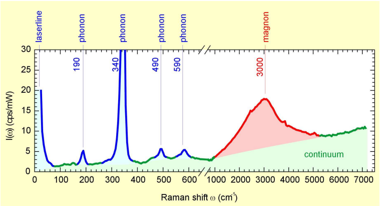
- struktura ukupne inducirane polarizacije $[\alpha(u) = \alpha_0 + \alpha' u + \dots]$

$$P_\alpha(\omega')\mathrm{e}^{-i\omega' t} = \chi_{\alpha\alpha}(\omega')E_\alpha(\omega')\mathrm{e}^{-i\omega' t} + \frac{\partial \chi_{\alpha\alpha}(\omega)}{\partial u} u\mathrm{e}^{i\omega_0 t} E_\alpha(\omega)\mathrm{e}^{-i\omega t}$$

- adijabatski izraz za konstantu vezanja

$$\delta\varepsilon_{\alpha\alpha}(\mathbf{x}, t) = 4\pi(\partial\chi_{\alpha\alpha}(\omega)/\partial u)u\mathrm{e}^{-i\mathbf{q}\cdot\mathbf{x} + i\omega_0 t}$$





Difrakcija X zraka

amplituda raspršenja iz FČS

- udarni presjek

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega'} = \left(\frac{e^2}{mc^2}\right)^2 \frac{1}{2}(1+\cos^2\theta')\langle|n(\mathbf{q})|^2\rangle$$

- amplituda raspršenja $A_{sc}(\mathbf{k},\mathbf{k}') = a(\mathbf{k},\mathbf{k}')\int_V \mathrm{d}^3x\,\mathrm{e}^{-i\mathbf{q}\cdot\mathbf{x}}n(\mathbf{x})$

$$A_{sc}(\mathbf{q}) = \sum_{nl}\mathrm{e}^{-i\mathbf{q}\cdot\mathbf{x}_{nl}}f_l(\mathbf{q}), \quad f_l(\mathbf{q}) = a(\mathbf{q})\int_V \mathrm{d}^3y\,\mathrm{e}^{-i\mathbf{q}\cdot\mathbf{y}}n_l(\mathbf{y})$$

- Braggova formula: $\mathbf{k} = \mathbf{k}' + \mathbf{K}_m$ ili $K_m = 2k\sin(\theta_m/2)$

$$A_{sc}(\mathbf{q}) = \sum_n \mathrm{e}^{-i\mathbf{q}\cdot\mathbf{R}_n}S(\mathbf{q}) = N\delta_{\mathbf{q},\mathbf{K}_m}S(\mathbf{K}_m), \;\; S(\mathbf{q}) = \sum_l f_l(\mathbf{q})\mathrm{e}^{-i\mathbf{q}\cdot\mathbf{r}_l^0}$$